

On the kinetic energy of unitary Fermi gas in a harmonic trap

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We have considered the orbital-free approximation of the kinetic energy functional to investigate the zero temperature properties of dilute harmonically trapped two component Fermi gas at unitarity. It is shown that our approach provides a reliable and inexpensive method to study superfluid strongly interacting dilute Fermi gases.

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The modern density functional theory (DFT) is based on the Kohn-Sham (KS) approach [1], where the noninteracting kinetic energy, T , is calculated in terms of the KS orbitals, although Ref.[2] proved the basic existence of functional $T(\rho)$, where ρ is the density, $\int \rho(\vec{r}) d^3r = N$, and N is the particle number. Since the numerical cost of self-consistently determining N orbitals rapidly increases for large N , the accurate density-functional approximation to the kinetic energy in terms of the density would reduce dramatically complexity of the DFT calculations (here we note the superfluid extension of the DFT given in Refs.[3-5]). There are various noninteracting kinetic energy functionals proposed in literature, for chemical applications see, for example, Refs.[6-21] (for nonlocal density functionals see Refs.[22-26]). For applications of the DFT to the nuclear structure physics see Ref.[27], web site, constructed for the universal nuclear energy density functional (UNEDF) collaboration, <http://unedf.org> and references therein.

The kinetic energy functional can be written as

$$T[\rho] = \frac{\hbar^2}{2m} \int \tau(\rho(\vec{r})) d^3r, \quad (1)$$

where the Kirgnitz semiclassical expansion for the kinetic energy density [28-31]

$$\tau(\rho(\vec{r})) = \tau_{TF}(\rho) + \frac{1}{9} \tau_W(\rho) + \dots, \quad (2)$$

where

$$\tau_{TF}(\rho) = \frac{3}{5} (3\pi^2)^{2/3} \rho^{5/3}, \quad (3)$$

is the well-known Thomas-Fermi (TF) kinetic energy density and $\tau_W(\rho)$ is the Weizsäcker kinetic energy density [12]

$$\tau_W(\rho) = [\vec{\nabla} \rho^{1/2}(\vec{r})]^2. \quad (4)$$

The semiclassical expansion (2) has to be considered as an asymptotic expansion [11]. While τ_{TF} is exact for the uniform gas model, $\tau_W(\rho)$ is considered exact in the limit of rapidly varying density ρ [13,14].

We present in this paper the simple linear combinations

$$\tau = \lambda_1(N) \tau_{TF} + \lambda_2(N) \tau_W \quad (5)$$

with λ_i determined empirically from the asymptotic region and for getting good energy of few fermion systems at unitarity. A N -dependence of λ_2 corresponds to the effective mass N -dependence [32].

There has been a lot of interest in systems of fermions at the unitarity [32-35] (when the scattering length diverges, the Bertsch many-body problem [36]). While Refs.[37-40] consider homogeneous systems, Refs.[41-45] present *ab initio* calculations of the properties of trapped fermionic atoms.

In Refs.[46,47] and later in Refs.[48-63] the dynamics of strongly interacting trapped dilute Fermi gases (dilute in the sense that the range of interatomic potential is small compared with inter-particle spacing) consisting of a 50-50 mixture of two different states is investigated in the single equation approach to the time-dependent density-functional theory, using $\lambda_1 = 1$ and a constant λ_2 approximations.

For the stationary case Eq.(5) leads to the following DFT equation

$$-\lambda_2(N) \frac{\hbar^2}{2m} \nabla^2 \Psi + V_{ext} \Psi + V_{xc} \Psi = \mu \Psi, \quad (6)$$

where $V_{xc}(\vec{r}) = [\frac{\partial \rho \epsilon(\rho)}{\partial \rho}]_{\rho=\rho(\vec{r})}$, $\epsilon(\rho)$ is the ground-state energy per particle of the homogeneous system, $\rho(\vec{r}) = |\Psi(\vec{r})|^2$ and μ is the chemical potential. For the remainder of this paper we will consider fermion systems at unitarity in a spherical harmonic trap

$$V_{ext}(\vec{r}) = \frac{m\omega^2 r^2}{2}. \quad (7)$$

The ground state energy is given by the minimum of the energy functional

$$J[\Psi] = \lambda_2(N) \frac{\hbar^2}{2m} \int \tau_W(\rho) d^3r + \int V_{ext} \rho d^3r + \int \epsilon(\rho) \rho d^3r, \quad (8)$$

where $\epsilon(\rho) = (\lambda_1(N) + \beta) 3\hbar^2 k_F^2 / (10m)$, $k_F = (3\pi^2 \rho)^{1/3}$, $\rho = |\Psi|^2$, and the universal parameter β [33] is estimated to be $\beta = -0.56$ [39].

To test the accuracy of approximation (5), we write the radial nonlinear equation (6) in asymptotic region

$$(-\lambda_2(N) \frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{r} + \lambda_2(N) \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} + \frac{m\omega^2 r^2}{2} - \mu) \Psi = 0. \quad (9)$$

The regular as $r \rightarrow \infty$ solution of Eq.(9) can be written as $z^{-3/4} W_{\kappa, l/2+1/4}(z)$, where W is the regular as $r \rightarrow \infty$ Whittaker function, $z = (m\omega / (\hbar \sqrt{\lambda_2(N)})) r^2$ and $\kappa = \mu / (2\hbar\omega \sqrt{\lambda_2(N)})$, therefore

$$\rho \sim e^{-z} z^{2\kappa-3/2}. \quad (10)$$

Since, in the limit of large r the Hartree-Fock density, $\rho_{HF}(\vec{r})$ is proportional to the square of the last occupied state

$$\rho_{HF}(\vec{r}) \sim e^{-m\omega r^2 / \hbar} r^{2\mu / (\hbar\omega) - 3}, \quad (11)$$

we expect that $\lim_{N \rightarrow \infty} \lambda_2(N) \rightarrow 1$. We also expect that $\lim_{N \rightarrow \infty} \lambda_1(N) \rightarrow 1$, since the TF kinetic energy density becomes exact in the large N limit. Note, that in the large r region the density is not slowly varying. For the kinetic energy functional in one spatial dimension Ref.[64] derived an upper bound

$$\langle \tau(\rho) \rangle \leq \langle \tau_W(\rho) \rangle + \langle \tau_{TF}(\rho) \rangle. \quad (12)$$

Although, the question whether the upper bound, Eq.(12), holds in the three dimensional case is still open question [65], our numerical results are in strong support of the inequality (12), see Fig. 1.

To study the effectiveness of the approximations (5) we calculate lower bounds to the ground state energy, Eq.(8), using the results of Ref.[62]

$$E^{(-)} = \frac{3}{2} \hbar \omega N \sqrt{\lambda_2(N) + \frac{3N^{2/3}(\lambda_1(N) + \beta)}{4}}. \quad (13)$$

To calculate upper bounds, $E^{(+)}$, we employing Fetter's trial functions [66]

$$\rho^{1/2}(\vec{r}) = b(1 - (1 - q)(dr)^2)^{1/(1-q)}, \quad (14)$$

where d and q are the variational parameters and b is the normalization constant, to minimize the functional J , Eq. (8).

Following Ref.[24], we propose the following approximation for the kinetic energy density, $\lambda_2 = 1$ and

$$\lambda_1(N) = (1 - \frac{1}{N})(1 - \frac{c}{N^\gamma}), \quad (15)$$

where c and γ are fixed by a least squares fit to the fixed-node diffusion Monte Carlo data [42], $c = 1.46832$, $\gamma = 0.78383$. It is clear from Table I that the fit is a very accurate. As for the lower $E^{(-)}$ and the upper $E^{(+)}$ bounds, they provide the actual solution of equation (6), $E = (E^{(+)} + E^{(-)})/2$ within $\pm\delta$ accuracy, with $\delta < 1\%$.

Recently, Refs.[58-60] have considered nonlinear equation, which for stationary case corresponds to the following approximation of the kinetic energy density

$$\tau = \frac{1}{4} \tau_W + \tau_{TF}. \quad (16)$$

Figures 2 and 3 show comparison between energy calculations using approximations (15), (16), (12) and the Thomas-Fermi approximation. It indicates that (i) there is a very good

agreement between calculations using (15) and (16) for $N/2 \geq 10$, (ii) the difference between all four approximations is negligible for $N/2 \geq 10^3$.

The $\tau = (1/4)\tau_W + \tau_{TF}$ approximation has incorrect asymptotic behavior for large r and N . The success of this approximation (see figures 2 and 3), however, indicates that the large r behavior have little or no consequence in the calculation of ground state energy of N fermion systems at unitarity in a spherical harmonic trap.

In conclusion, we summarize the main points of this paper.

- (i) We have considered the orbital free approximation of the kinetic energy functional, proposed for the first time by Acharya et al. [19], to investigate N -fermion systems at unitarity consisting of 50-50 mixture of two different states and confined in a spherical harmonic trap.
- (ii) We found that our analytical lower bound, Eq.(13), describes the ground state energy with a very good accuracy, providing an easy and simple quantitative tool for trapped Fermi gases, without relying on complex and extensive computations.

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Table I. The energies $E^{(-)}$, Eq. (), $E^{(+)}$, $E = (E^{(-)} + E^{(+)})/2$ and the energy calculated within the fixed-node diffusion Monte Carlo method, E^{MC} [42], all in units of $\hbar\omega$ for $N \leq 30$ [see the text for further details].

$N/2$	$E^{(-)}$	$E^{(+)}$	E^{MC}	E
4	12.47	12.51	12.58	12.49
5	16.69	16.82	16.81	16.76
6	21.20	21.43	21.28	21.31
7	25.95	26.29	25.92	26.12
8	30.92	31.37	30.88	31.15
9	36.09	36.66	35.97	36.38
10	41.45	42.14	41.30	41.80
11	46.98	47.80	46.89	47.39
12	52.67	53.61	52.62	53.14
13	58.52	59.58	58.55	59.05
14	64.51	65.70	64.39	65.10
15	70.63	71.95	70.93	71.29

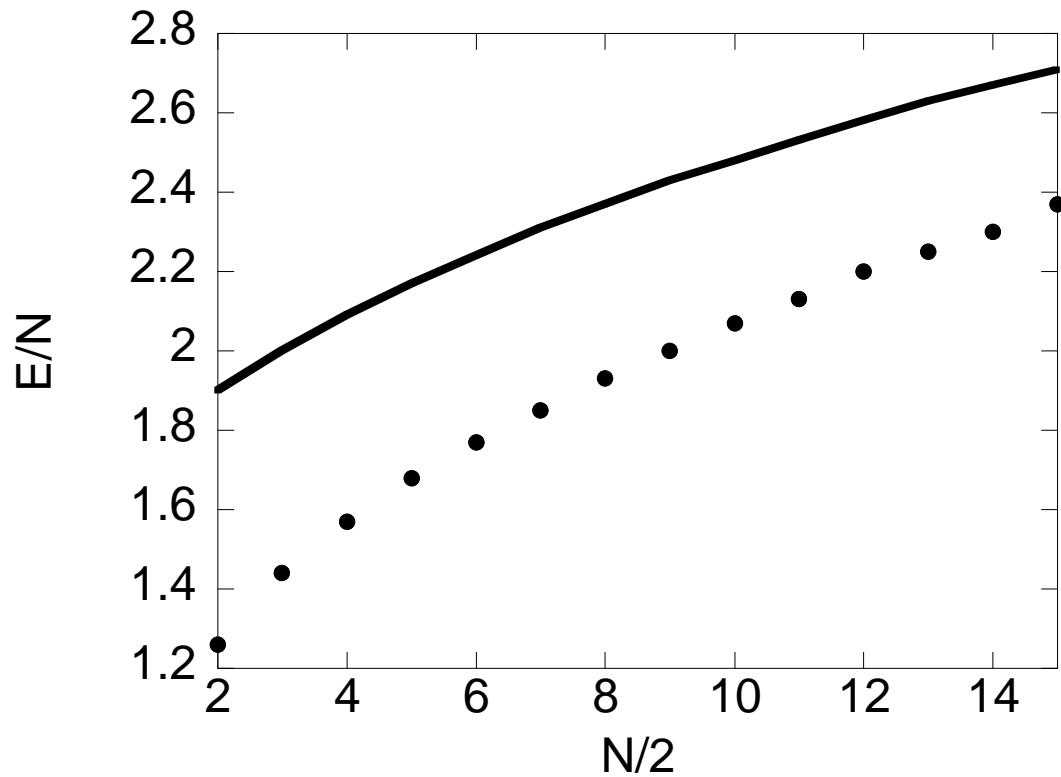


Fig.1. Ground state energy per particle of few-fermion systems at unitarity in a spherical harmonic trap in units of $\hbar\omega$ as a function of number of atoms N . The solid line represents $\tau = \tau_{TF} + \tau_W$ approximation. The circular dots indicate results of Ref.[42].

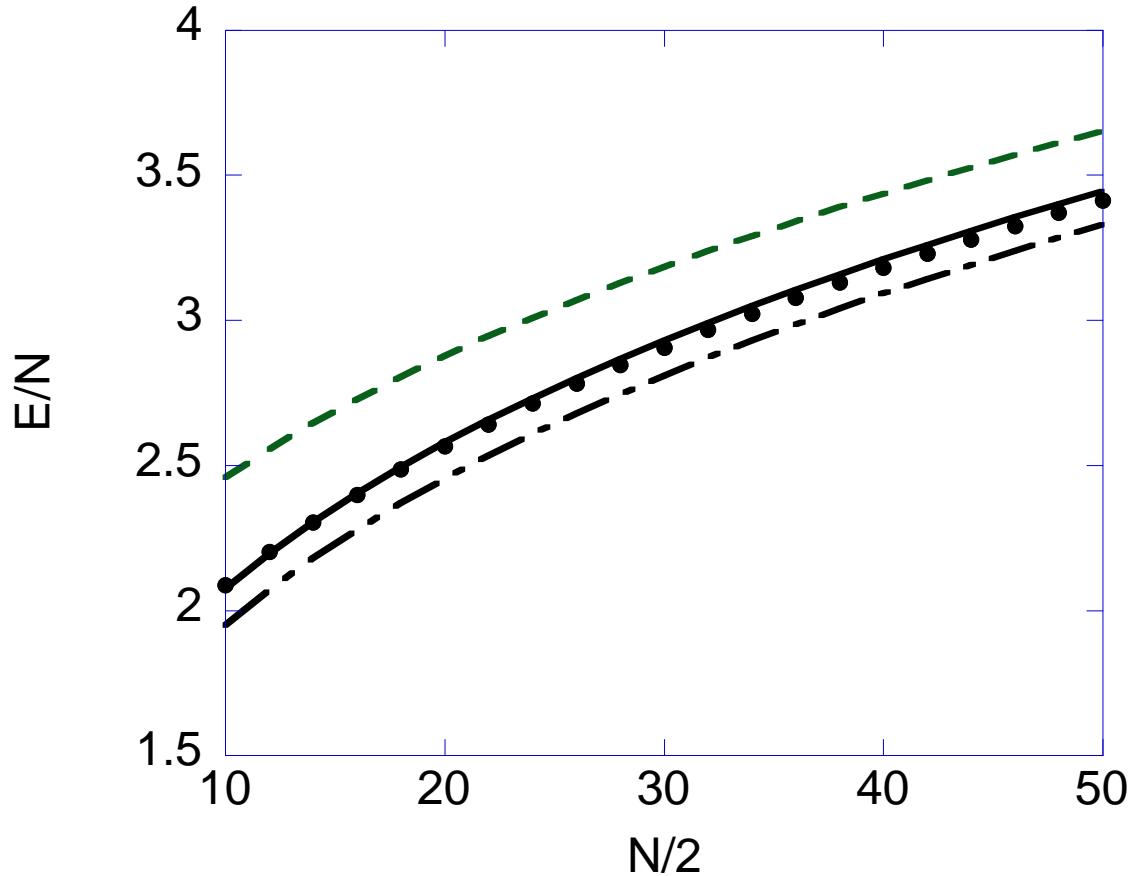


Fig.2. Ground state energy per particle in units of $\hbar\omega$ as a function of number of atoms N . The solid line, the circular dots, the dashed line and the dashed-dotted line represent results calculated using $\tau = \tau_W + \lambda_1(N)\tau_{TF}$, $\tau = (1/4)\tau_W + \tau_{TF}$, $\tau = \tau_W + \tau_{TF}$ and $\tau = \tau_{TF}$ approximation, respectively.

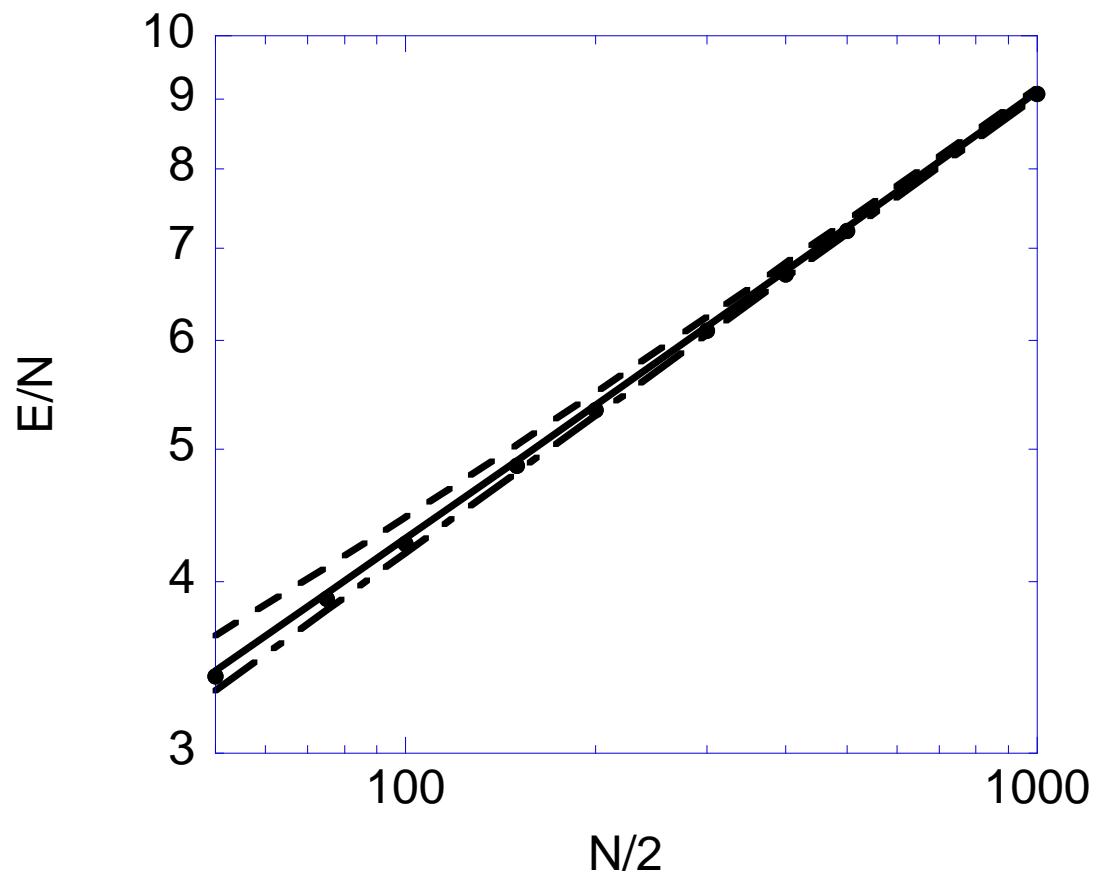


Fig.3. Same as in Fig. 2.

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